



# AQUATOX – A Modular Fate and Effects Model for Aquatic Ecosystems – Release 1.1: Volume 2 – Technical Documentation (Addendum)

*Since its first release by EPA in September 2000, there have been several changes made to AQUATOX, most significantly those that have improved the simulation of periphyton (attached algae) in streams and rivers. Minor enhancements were also made which improve simulation of macrophytes, fish, and dissolved oxygen. A typographic error was discovered in the documentation relating to volatilization; the model code was correct. This addendum presents the specific changes to the Technical Documentation (EPA document number 823-R-01-007).*

## **Periphyton**

***The following should replace “Washout and Entrainment” on pp. 4-17 and 4-18)***

### **Washout and Sloughing**

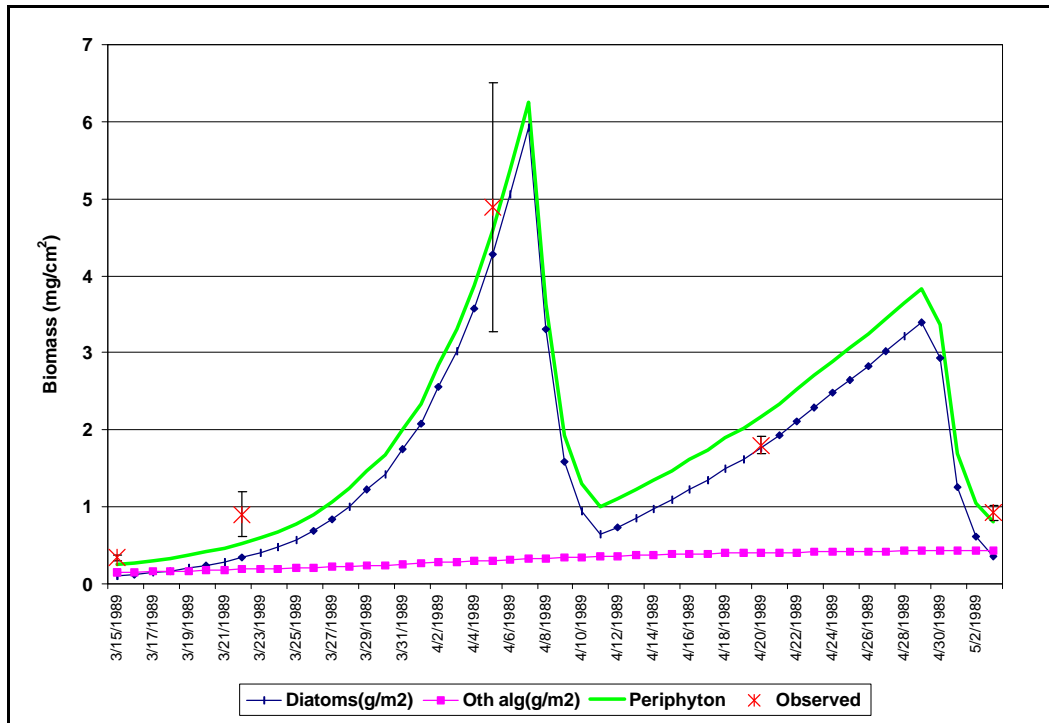
Phytoplankton are subject to downstream drift. In streams and in lakes and reservoirs with low retention times this may be a significant factor in reducing or even precluding phytoplankton populations (LeCren and Lowe-McConnell, 1980). The process is modeled as a simple function of discharge:

$$Washout_{phytoplankton} = \frac{Discharge}{Volume} \cdot Biomass$$

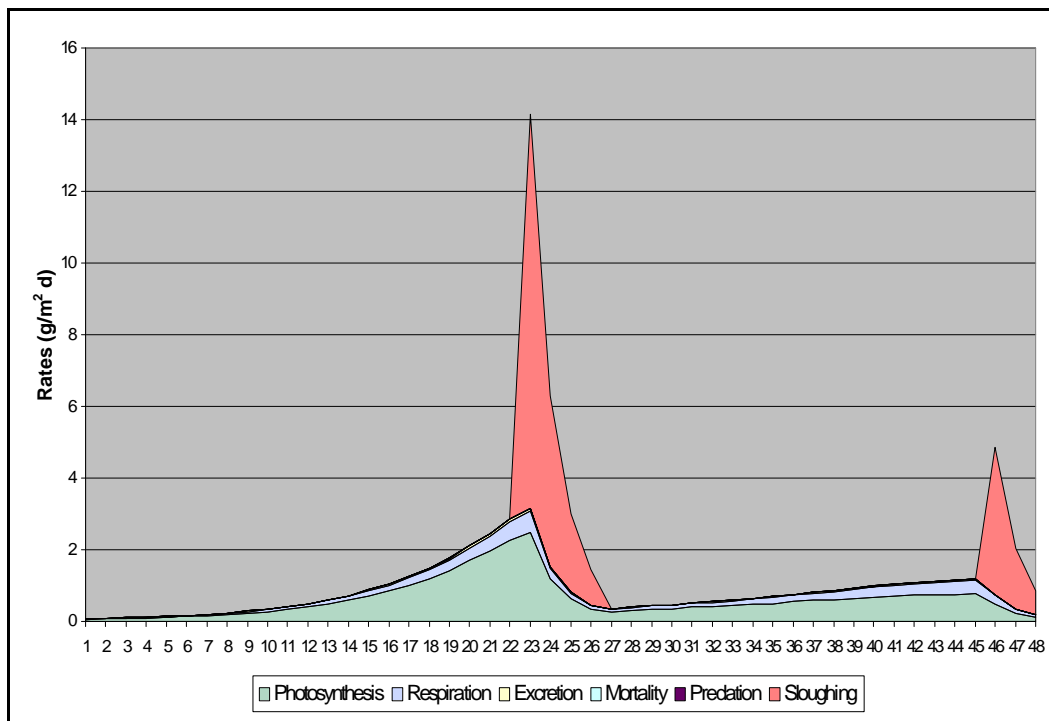
where:

<i>Washout</i>	=	loss due to downstream drift (g/m <sup>3</sup> d),
<i>Discharge</i>	=	daily discharge (m <sup>3</sup> /d);
<i>Volume</i>	=	volume of site (m <sup>3</sup> ); and
<i>Biomass</i>	=	biomass of phytoplankton (g/m <sup>3</sup> ).

Periphyton may also lose biomass due to high stream velocity. Originally AQUATOX modeled this as entrainment, being a function of stream discharge and biomass. Attempts at calibration for periphyton using a high quality data set were unsuccessful because they were unable to reproduce the buildup and then decline in periphyton biomass. As a result, the formulation for entrainment was reexamined and a more complex sloughing formulation, extending the approach of Asaeda and Son (2000), was implemented. This function was able to represent a wide range of conditions better (**Figure 1** and **Figure 2**).



**Figure 1.** Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of both N and P and removal of grazers in Spring, 1989.



**Figure 2.** Predicted rates for diatoms in Walker Branch, Tennessee, with addition of both N and P and removal of grazers in Spring, 1989. Note the importance of periodic sloughing.

Sloughing is a function of senescence due to suboptimal conditions and the drag force of currents acting on exposed biomass. Drag increases as both biomass and velocity increase:

$$DragForce = Rho \cdot DragCoeff \cdot Vel^2 \cdot (BioVol \cdot UnitArea)^{2/3} \cdot 1(E-6)$$

where:

<i>DragForce</i>	=	drag force (kg m/s <sup>2</sup> );
<i>Rho</i>	=	density (kg/m <sup>3</sup> );
<i>DragCoeff</i>	=	drag coefficient (2.53E-4, unitless);
<i>Vel</i>	=	velocity (m/s);
<i>BioVol</i>	=	biovolume of algae (mm <sup>3</sup> /mm <sup>2</sup> );
<i>UnitArea</i>	=	unit area (mm <sup>2</sup> );
1E-6	=	conversion factor (m <sup>2</sup> /mm <sup>2</sup> ).

Biovolume is not modeled directly by AQUATOX, so a simplifying assumption is that the empirical relationship between biomass and biovolume is constant for a given growth form, based on observed data from Rosemond (1993):

$$BioVol_{Dia} = \frac{Biomass}{2.08E-9}$$

$$BioVol_{Fil} = \frac{Biomass}{8.57E-9}$$

where:

<i>BioVol<sub>Dia</sub></i>	=	biovolume of diatoms (mm <sup>3</sup> /mm <sup>2</sup> );
<i>BioVol<sub>Fil</sub></i>	=	biovolume of filamentous algae (mm <sup>3</sup> /mm <sup>2</sup> );
<i>Biomass</i>	=	biomass of given algal group (g/m <sup>2</sup> ).

Suboptimal light and nutrients cause senescence of cells that bind the periphyton and keep them attached to the substrate. This effect is represented by a factor, *Suboptimal*, which is computed in modeling the effects of suboptimal nutrients and light on photosynthesis, and which is multiplied by 5 to desensitize its effect on sloughing. *Suboptimal* decreases the critical force necessary to cause sloughing. If the drag force exceeds the critical force for a given algal group modified by the *Suboptimal* factor, then sloughing occurs:

$$\text{If } DragForce > Suboptimal_{Org} \cdot FCrit_{Org} \text{ then } Slough = Biomass \cdot FracSloughed \\ \text{else } Slough = 0$$

where:

<i>Suboptimal<sub>Org</sub></i>	=	factor for suboptimal nutrient and light effect on senescence of given periphyton group (unitless);
<i>FCrit<sub>Org</sub></i>	=	critical force necessary to dislodge given periphyton group (kg m/s <sup>2</sup> );
<i>Slough</i>	=	biomass lost by sloughing (g/m <sup>3</sup> );
<i>FracSloughed</i>	=	fraction of biomass lost at one time (90%, unitless).

$$Suboptimal_{Org} = NutrLimit_{Org} \cdot LtLimit_{Org} \cdot 5$$

$$\text{If } Suboptimal_{Org} > 1 \text{ then } Suboptimal_{Org} = 1$$

where:

*NutrLimit* = nutrient limitation for given algal group (unitless) computed by AQUATOX;  
*LtLimit<sub>Org</sub>* = light limitation for given algal group (unitless) computed by AQUATOX.

## Detrital Accumulation in Periphyton

In phytoplankton, mortality results in immediate production of detritus, and that transfer is modeled. However, for purposes of modeling, periphyton are defined as including associated detritus. The accumulation of non-living biomass is modeled implicitly by not simulating mortality due to suboptimal conditions. Rather, in the simulation biomass builds up, causing increased self-shading, which in turn makes the periphyton more vulnerable to sudden loss due to sloughing. The fact that part of the biomass is non-living is ignored as a simplification of the model, with compensation through the high internal extinction rate constant.

## Macrophytes

*The following equation should replace Eq. 64 on p. 4-19:*

$$\frac{dBiomass}{dt} = Loading + Photosynthesis - Respiration - Excretion - Mortality - Predation - Breakage \quad (6)$$

*In the list of definitions for the above variables on p. 4-20, “Washout” should be replaced by:*

*Breakage* = loss due to breakage (g/m<sup>2</sup>d)

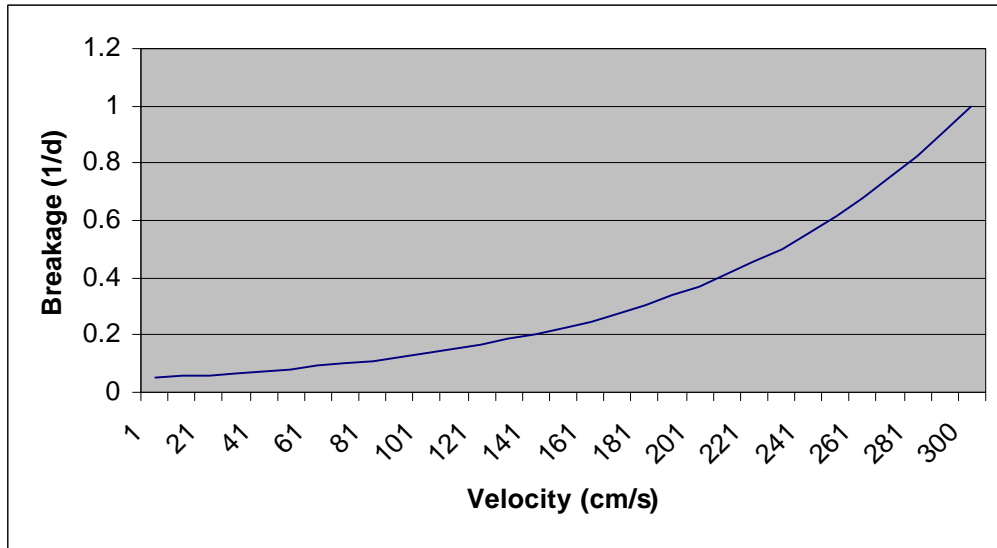
*The following should be inserted after Figures 40 and 41 on p. 4-21 :*

Macrophytes are subject to breakage due to higher water velocities; this breakage of live material is different from the sloughing of dead leaves. Although breakage is a function of shoot length and growth form as well as currents (Bartell et al., 2000; Hudon et al., 2000), a simpler construct was developed for AQUATOX (**Figure 3**):

$$Breakage = \frac{Velocity - VelMax}{Gradual \cdot UnitTime} \cdot Biomass$$

where:

*Breakage* = macrophyte breakage (g/m<sup>2</sup> d);  
*Velocity* = current velocity (cm/s);  
*VelMax* = velocity at which total breakage occurs (300 cm/s);  
*Gradual* = velocity scaling factor (100 cm/s);  
*UnitTime* = unit time for simulation (1 d);  
*Biomass* = macrophyte biomass (g/m<sup>2</sup>).



**Figure 3.** Breakage of macrophytes as a function of current velocity.

### **Fish**

***The following should be inserted in place of Eq. 77 in “Respiration” on p. 4-27:***

Respiration in fish increases with crowding due to competition for spawning sites, interference in feeding, and other factors. This adverse intraspecific interaction helps to constrain the population to the carrying capacity; as the biomass approaches the carrying capacity for a given species the respiration is increased proportionately (Kitchell et al., 1974):

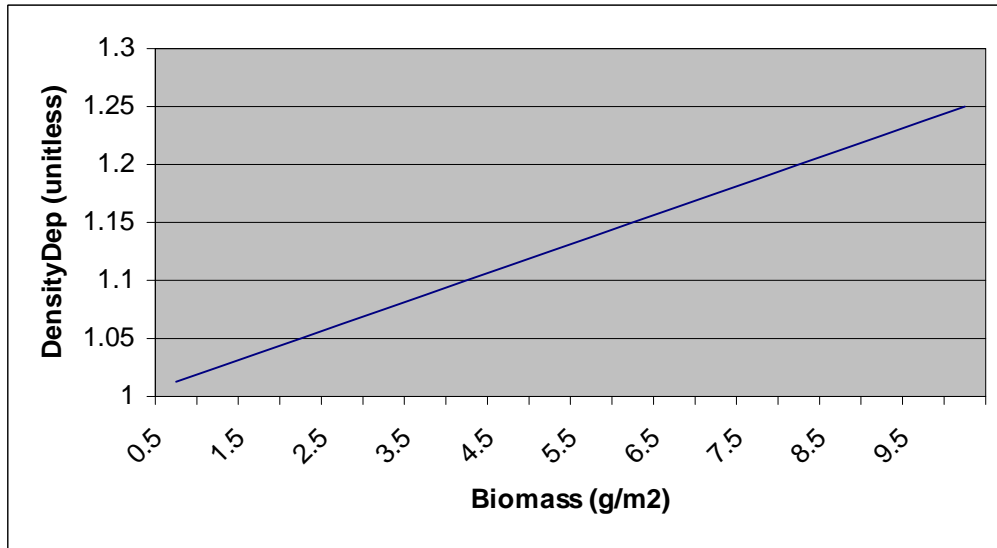
$$Endogenous_{pred} = EndogResp_{pred} \cdot TCorr_{pred} \cdot Biomass_{pred} \cdot DensityDep$$

$$DensityDep = 1 + \frac{IncrResp \cdot Biomass}{KCap}$$

where:

$Endogenous_{pred}$	=	basal respiratory loss modified by temperature and crowding (g/m <sup>3</sup> d);
$EndogResp_{pred}$	=	basal respiration rate at 0° C for given animal (1/day); parameter input by user as “Respiration Rate;”
$TCorr_{pred}$	=	Stroganov temperature function (unitless);
$Biomass_{pred}$	=	concentration of organism (g/m <sup>3</sup> ).
$DensityDep$	=	density-dependent respiration factor used in computing endogenous respiration (unitless);
$IncrResp$	=	increase in respiration at carrying capacity (0.25);
$KCap$	=	carrying capacity (g/m <sup>3</sup> ).

With the *IncrResp* value of 0.25, which is a conservative estimate, respiration is increased by 25% at carrying capacity (Kitchell et al., 1974), as shown in **Figure 4**. Note that the same equation is used for invertebrates; but, by setting a high carrying capacity, density dependence is not an important factor for invertebrates.



**Figure 4.** Density-dependent factor for increase in respiration as fish biomass approaches the carrying capacity (10.0 in this example).

### Oxygen Transfer

*The following should be inserted after Eq. 139, and its accompanying definitions, on p. 5-17:*

Algal blooms can generate dissolved oxygen levels that are as much as 400% of saturation (Wetzel, 2001). However, near-surface blue-green algal blooms, which are modeled as being in the top 0.25 m, produce high levels of oxygen that do not extend significantly into deeper water. An adjustment is made in the code so that if the blue-green algal biomass exceeds 1 mg/L and is greater than other phytoplankton biomass, the thickness subject to oxygen reaeration is set to 0.25 m. This does not affect the  $K_{Reaer}$  that is used in computing volatilization.

### Volatilization

*There was a typographic error discovered in Eq. 178, which should be replaced with the following (replacing “- Volatilization” with “+ Volatilization”):*

$$\begin{aligned}
 \frac{dToxicant_{Water}}{dt} = & Loading + \sum_{LabileDetr} (Decomposition_{LabileDetr} \cdot PPB_{LabileDetr} \cdot 1e-6) \\
 & + \sum Desorption_{DetrTox} + \sum_{Org} (K2 \cdot PPB_{Org} \cdot 1e-6) \\
 & - \sum Sorption_{DetrTox} - \sum GillUptake_{Pred} - MacroUptake \\
 & - \sum AlgalUptake_{Alga} - Hydrolysis - Photolysis - MicrobialDegrn \\
 & + Volatilization - Discharge + TurbDiff
 \end{aligned}$$

***The following note should be inserted on page 7-15, following Eq. 209 and its accompanying list of definitions:***

Because theoretically toxicants can be transferred in either direction across the water-air interface, Eq. 209 is formulated so that volatilization takes a negative sign when it is a loss term.

### **References**

- Asaeda, T., and D.H. Son. 2000. Spatial structure and populations of a periphyton community: a model and verification. *Ecological Modelling*, 133:195-207.
- Rosemond, A.D. 1993. *Seasonality and Control of Stream Periphyton: Effects of Nutrients, Light, and Herbivores*. Dissertation, Vanderbilt University, Nashville, Tenn., 185 pp.
- Bartell, S.M., K.R. Campbell, E.P.H. Best, and W.A. Boyd. 2000. *Ecological Risk Assessment of the Effects of the Incremental Increase of Commercial Navigation Traffic (25, 50, 75, and 100% Increase of 1992 Baseline Traffic) on Submerged Aquatic Plants in the Main Channel and Main Channel Borders*. ENV Report 17, prepared for U.S. Army Engineer District, Rock Island, U.S. Army Engineer District, St. Louis, U.S. Army Engineer District, St. Paul. 109 pp.
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- Kitchell, J.F., J.F. Koonce, R.V. O'Neill, H.H. Shugart, Jr., J.J. Magnuson, and R.S. Booth. 1974. Model of Fish Biomass Dynamics. *Trans. Am. Fish. Soc.* 103:786-798.
- Wetzel, R.G. 2001. *Limnology: Lake and River Ecosystems*. San Diego: Academic Press, 1006 pp.